Moving Toward an Atomistic Reader Model

E. D. Boerner, O. Chubykalo-Fesenko, O. N. Mryasov, R. W. Chantrell, and O. Heinonen

***Abstract*—With the move to recording densities up to and beyond 1 Tb/in^2, the size of read elements is continually reducing as a requirement of the scaling process. The expectation is for read elements containing magnetic films as thin as 1.5 nm, in which finite size effects, and factors such as interface mixing might be expected to become of increasing importance. Here, we review the limitations of the current (micromagnetic) approach to the theoretical modeling of thin films and develop an atomistic multiscale model capable of investigating the magnetic properties at the atomic level. Finite-size effects are found to be significant, suggesting the need for models beyond the micromagnetic approach to support the development of future read sensors.**

***Index Terms*—Atomistic calculations, computational modeling, read elements.**

I. Introduction

HISTORICALLY, conventional magnetic recording has been characterized by a trend of increasing storage density. This has been achieved by a continuous scaling of materials properties such as the coercivity and medium grain size, and of component sizes, particularly the read and write tranducers. Although it seems likely that a step change in the recording technology from the longitudinal to the perpendicular mode will occur in the near future, the scaling process must continue if the areal density progress is to continue. This process presents a number of technical and physical challenges, and it is clear that advanced modeling techniques will be necessary in order to understand the materials and device physics and the consequent design implications. However, device sizes are entering the regime in which finite-size effects are expected to become important. For example, it was first pointed out by Smith and Arnett [1] that thermally induced magnetization fluctuations would become an increasingly important noise source as the dimensions of read heads are reduced. This arises from simple thermodynamic considerations assuming that the magnetic element can be considered a single domain. However, an equally fundamental problem arises from the fact that film thicknesses are approaching atomic dimensions. Short-term developments demand film thicknesses on the order of 3 nm and scaling arguments lead to the requirement of a reduction of this value to around 1.5 nm. At these dimensions, it is reasonable to conjecture that finite size effects may begin to play an important role in the magnetic and transport behavior of the devices themselves. These considerations lead to a need to analyze the suitability of the currently available models. In this paper, we consider the limitations of current models and propose a new formalism based on an atomistic approach, which, although at an early stage, is potentially capable of device simulations from a very fundamental level, including finite size effects explicitly. We first consider the micromagnetic formalism and its limitations, and outline the atomistic approach before considering some static and dynamic calculations on thin film elements which demonstrate important finite size effects on the magnetic properties.

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II. Micromagnetics and the Landau–Lifshitz–Gilbert (LLG) Equation

The modeling approach currently used is based on the formalism of micromagnetics, which is very successful in understanding basic magnetization processes and the origin of magnetic noise in read elements. The formalism of micromagnetics as developed by Brown [2] employs a combination of energy minimization and classical nucleation theory to predict the stationary states and nucleation fields of systems large enough to exhibit nonuniform magnetization states. The total energy to be minimized is considered to be a sum of the exchange, magnetostatic, anisotropy, and Zeeman terms. Of these, the most problematic is the magnetostatic term, because of its long-range nature. Micromagnetics takes the approach of solving the magnetostatic problem (in principle exactly) using a continuum model in which the magnetization is considered to be a spatially continuous vector field. However, this forces a long-wavelength approximation on the exchange term. Essentially, we start with some atomic scale representation of the exchange, most commonly the Heisenberg form, in which the exchange energy of spin Si is given (see, for example, [3]) by

$$E_j^{\text{exch}} = -\sum_{i \neq j} J_{ij} \hat{S}_i \cdot \hat{S}_j \tag{1}$$

where the sum is often taken over nearest neighbors only, given the short-range nature of the exchange. Under the assumption of small angular changes between individual spins on neighboring atoms (corresponding to the approximation of long-wavelength magnetization fluctuations), it is straightforward to show that the exchange energy locally is given by

$$E^{\text{exch}}(\vec{r}) = A(\nabla M)(\vec{r}))^2 \tag{2}$$

where for a simple cubic lattice $A = 2JS^2/a$ with a the lattice constant. The total exchange energy is given by an integration over $(\vec{r})$. We note that the atomic level information has become absorbed into the constant A.

During the past 15 years or so, there has been a continuous process of developing improved mathematical and computational techniques for the calculation of the magnetostatic field, which is the most time consuming aspect of numerical approaches to micromagnetics. However, developments of the physical basis of the formalism have been less numerous, and here we will mention the two major developments relevant

to the current paper. First, the basic formulation of micromagnetics gives only stationary states (before nucleation), the nucleation field, and the mode of magnetization reversal. Equally important for complex magnetization processes is the determination of the magnetic state after magnetization reversal. Given the complexity of the energy surface in realistic cases, the final magnetization state can only be determined by consideration of the dynamic path of the magnetization during the reversal process. Dynamic calculations were first made by Victora [4] using the LLG equation

$$\frac{d\hat{m}}{dt} = \gamma_0 \hat{m} \times \vec{H} - \alpha\gamma_0 \hat{m} \times \vec{H} \times \vec{H} \tag{3}$$

where $\hat{M}$ is the unit vector and γ_0 is the gyromagnetic ratio. α is a phenomenological damping constant. The second development of importance is the introduction of thermal activation into the micromagnetic formalism [5], [6]. The micromagnetic formalism is intrinsically athermal, with magnetization reversal taking place at 0 K. The introduction of thermally activated magnetization reversal leads to a thermodynamically consistent formalism, allowing finite temperature reversal processes to be simulated. The theory is based on the work of Brown [7]. It is assumed that thermal effects can be represented by a random field having a Gaussian distribution with zero magnitude and a variance given by

$$\mu = \frac{2kT\alpha}{VM_s\gamma(1-\alpha^2)\Delta t} \tag{4}$$

where Δt is the time step, M_s is the saturation magnetization of the material, and V is the particle volume. Numerically, it is easy to determine an instantaneous thermal field from (4). Adding this field to the LLG equation produces the Langevin equation of the problem, for which reason the approach is often referred to as the Langevin dynamic (LD) technique. The resulting stochastic differential equation can be solved, for example, using the Heun method [8] which leads to the Stratonovitch solution.

Using the LD approach is not only important for the simulation of magnetization reversal processes. Smith and Arnett [1] first suggested that as device sizes reduce, thermally activated magnetization fluctuations will become an increasingly important source of noise. This effect has been studied numerically [9]–[12]. Although the effects of spin momentum transfer were found to be important in [10], more recent work [11], [12] has shown that the origin of magnetic noise can also have a purely micromagnetic origin, arising from fluctuations of the magnetization between two metastable states. Here, we note that the thermal activation is added in a long-wavelength approximation. Previous approaches to try to use the micromagnetic formalism to simulate the variation of magnetization with temperature [13] have been unsuccessful essentially because this approach does not introduce the short-wavelength fluctuations which are central to the M versus T variation. It is possible that the coupling between the short- and long-wavelength modes will have a bearing on the magnetic noise, and atomistic multiscale calculations are the most promising way to answer such questions. In this paper, we present a simple multiscale atomistic model of thin film elements and apply the model to calculations of magnetization reversal and magnetization fluctuations in thin film elements.

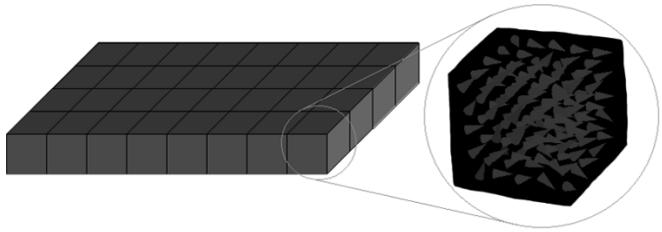

Fig. 1. Schematic diagram of the magnetostatic field calculation. The magnetic moment is averaged over the spins within a cell of the superlattice and the averaged moments are use to calculate the local magnetostatic field.

III. Model

The approach used is to base the calculation at the atomic rather than micromagnetic lengthscale. That is, our computational cell uses atomic level discretization. As a result, we can use some physically reasonable form for the exchange interaction. Here, we use the Heisenberg form (1). The use of (1) means that we treat accurately exchange contribution to the short-wavelength fluctuations responsible for the magnetic phase transition. However, this leaves the necessity of calculating the (long-range) magnetostatic term, which can be calculated very efficiently within the usual micromagnetic approach. Of course it is still possible to carry out the calculation of the magnetostatic field exactly, using, for example, the FFT approach at the atomic level. However, this is very time consuming. Here, we use an alternative multiscale approach, in which we approximate the magnetic field by averaging the magnetic moments on a regular superlattice and then use the FFT technique to calculate the resulting magnetic field.

The calculation is shown schematically in Fig. 1. Essentially, the magnetization is averaged over each cell within the superlattice and it is this structure of macroscopic magnetic moments which is used to calculate the field. We note that this approach averages out the fluctuations in the magnetostatic field over the atomic lengthscale. However, on this lengthscale the fluctuations in the exchange field are expected to be dominant, and the neglect of short-wavelength magnetostatic field fluctuations is unlikely to have a significant effect on the atomic level properties such as the saturation magnetization. This approach significantly speeds up the calculation of the magnetostatic field, to the extent that it is possible to simulate ensembles containing in excess of 10^6 spins on a single processor. Here, we present calculations using both Monte Carlo (MC) and LD methods. MC calculations in principle simulate static rather than dynamic processes. However, it has been shown [14] that the timescale in MC steps can be directly related to the physical time, at least for timescales much longer than the precession frequency. For the LD calculations, (4) is simply modified by replacing the moment of the particle (M_sV) by the atomic magnetic moment μ.

IV. Results

A. Finite Size Effects and Magnetization Fluctuations in Nanowires and Platelets

We first present some results on calculations of magnetization fluctuations in platelets in order to test the model in calculations of magnetization reversal. All calculations in this section were carried out using the MC model. Typical results are given for a platelet of dimensions (x, y, z) 45 nm $\times$ 45 nm $\times$ 1.5 nm.

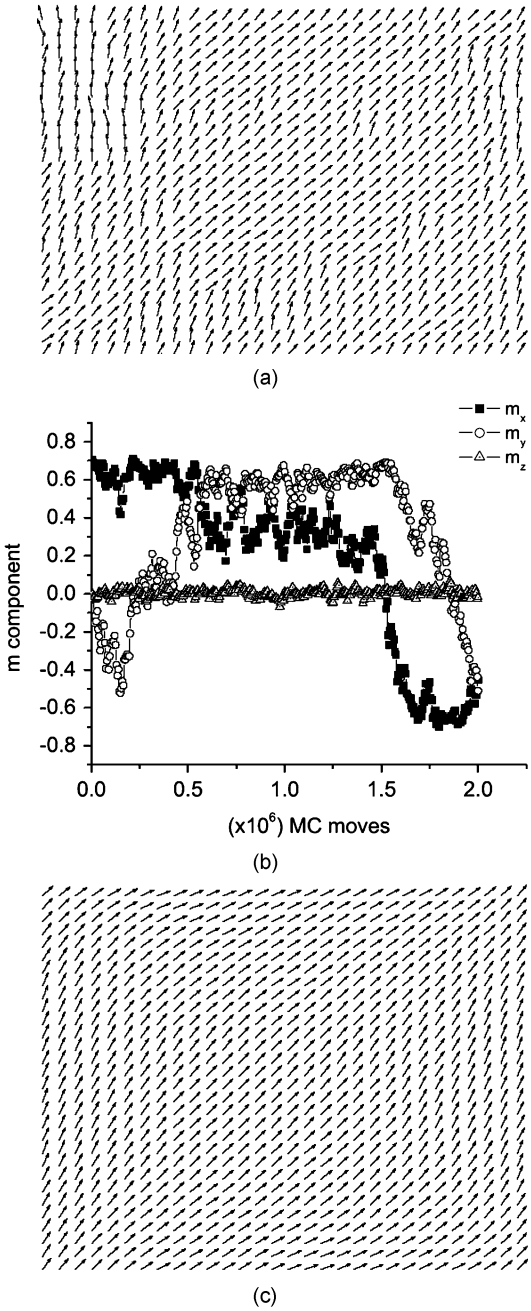

Fig. 2. (a) Leaf state for a 45 × 45 nm × 1.5 nm platelet. The magnetization fluctuates between minima along the diagonals of the platelet. (b) The variation of the magnetization with the number of MC moves per spin. (c) The leaf state at a temperature of 10 K.

The material is assigned zero crystalline anisotropy, hence the net anisotropy arises entirely from shape. The calculations are made at 300 K and the assumed value of J gives $T_c = 600$ K. The atomic spins are initially aligned in the direction of the short axis, i.e., the hard axis of the platelet. After several hundred Monte Carlo steps per spin (MCS), the magnetization rotates along the easy axis of the platelet due to the effective shape anisotropy arising from the magnetostatic field. The magnetization forms a leaf-like state as shown in Fig. 2(a), with an easy magnetization direction along the platelet diagonal as expected from the configurational anisotropy. However, due to the thermal effects and the relatively low energy barriers involved, the easy (diagonal) magnetization directions are

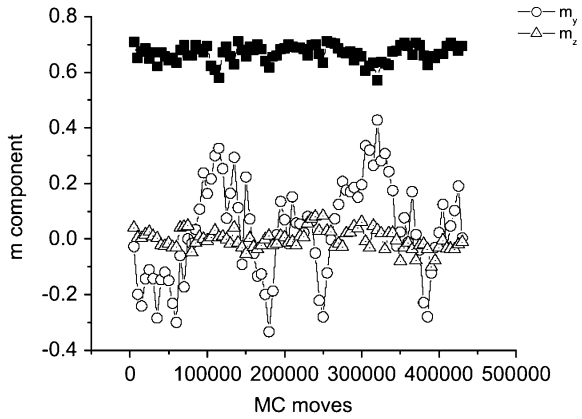

Fig. 3. Magnetization components for a 45 × 15 × 1.5 nm element showing stability of the magnetization along the easy axis.

metastable, and the magnetization is able to surmount the energy barrier and rotate readily between easy directions. This is demonstrated in Fig. 2(b), which shows the variation of the magnetization components with the number of Monte Carlo steps. It can be seen that there are magnetization transitions between states close to the energy minima resulting from the configurational anisotropy. Thus, at the macroscopic level, the multiscale model predicts similar behavior to that expected from micromagnetics. This is also indicated in Fig. 2(c), which shows calculations at the lower temperature of 10 K. The reduction in temperature results, as expected, in smaller local magnetization fluctuations and stability of the magnetization along an easy axis of the configurational anisotropy.

The introduction of some shape anisotropy can of course stabilize the magnetization, as shown in Fig. 3, which shows the evolution of the magnetization components as a function of the number of MC steps per spin for a 45 × 15 × 1.5 nm element. The magnetization fluctuates as expected about the long (x) axis of the element.

Thus, the atomistic model reproduces qualitatively similar behavior to micromagnetics. The greater significance of the atomistic approach is first apparent in the effects of the finite thickness on the magnetization structure. Fig. 4 shows the magnetization components at $T = 300$ K for a platelet of dimensions 45 × 45 × 1.5 nm, for a material with $T_c = 650$ K. The system was first allowed to reach equilibrium and then allowed to evolve for a further 13 000 moves. In Fig. 4 we show the total magnetization $m_{\rm tot}$, and magnetization of the surface plane of atoms $m_{\rm surface}$ and of the central plane of atoms $m_{\rm center}$. While the magnetization of the central plane of atoms is close to the calculations for the bulk material (0.73), the outer plane of atoms has a magnetization reduced by approximately 10% of the bulk value. It is reasonable to suppose that this magnetization variation should have some bearing on the transport properties of the film, although this is beyond the scope of the current work. However, finite-size effects on the transport properties would seem to be a significant consideration for future reader designs, and it should be stressed that the investigation of this phenomenon is outside the scope of micromagnetics.

B. Dynamic Calculations and Magnetization Fluctuations

We have used the atomistic model to carry out dynamic simulations using the LD approach including a local magnetic field derived from the classical spin Hamiltonian. We first apply the

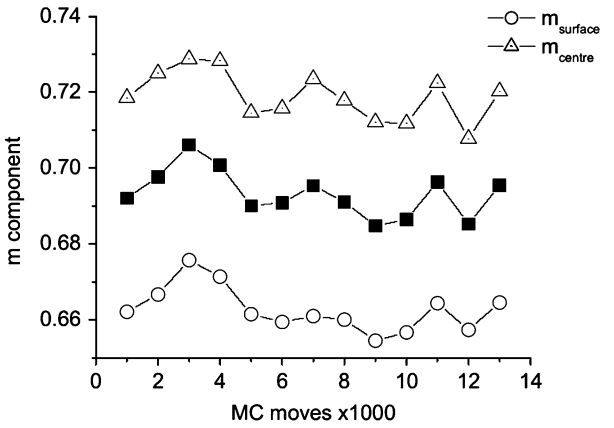

Fig. 4. Magnetization components for a $45 \times 45 \times 1.5$ nm platelet. There is a reduction of the magnetization in the surface planes.

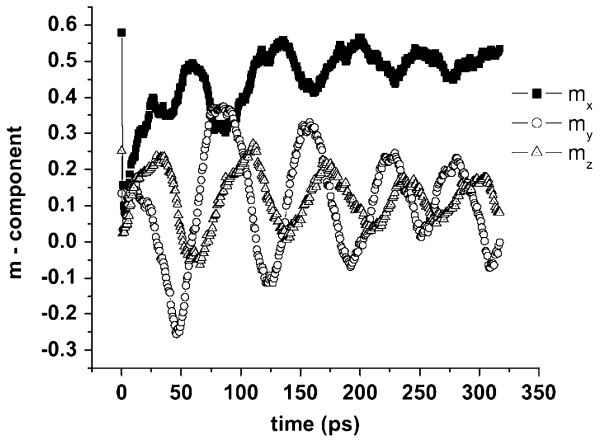

Fig. 5. Magnetization components for a $15 \times 15 \times 1.5$ nm Fe platelet during and after the application of a 100 ps laser pulse.

model to the simulation of pump–probe dynamic measurements. Here, a field is applied at an angle of 45° to a thin film sample, in this case consisting of a $15 \times 15 \times 1.5$ nm Fe platelet, and taking a damping constant of $\alpha = 0.1$. The sample is heated with a laser pulse of duration 100 ps, consequently reducing the magnitude of the magnetization. As the magnetization recovers after the laser pulse, it follows a precessional motion back to the original equilibrium position.

The results are given in Fig. 5. On application of the laser pulse, there is an initial rapid decrease in the magnetization from the $T = 300$ K spontaneous magnetization to a value close to zero. Note that this initial loss of magnetization occurs extremely rapidly, which is consistent with experimental data. After the laser pulse is switched off the magnetization recovers rather more slowly, as will be discussed in more detail elsewhere. Most importantly in the context of the current paper, the dynamic atomistic approach using the LLG equation reproduces qualitatively the behavior observed experimentally. Specifically, the rapid loss and slow recovery of the magnetization is followed by a transition to a damped precessional regime, with the initial magnetization state recovered after several hundred picoseconds. Pump–probe experiments are an important test of the dynamic model, and in the long-term a detailed comparison with experiment is expected to lead to improved understanding of damping processes in magnetic materials.

Clearly the atomistic model might be expected to exhibit fluctuations of the magnetization on lengthscales typical of a micromagnetic discretization cell. This is of relevance to our comparison with micromagnetic calculations since the micromagnetic formalism does not include such fluctuations of the magnetization. Here, we present dynamic calculations of the magnetization in Fe cubes of size $1.5 \times 1.5 \times 1.5$ nm and $3 \times 3 \times 3$ nm. The calculations are carried out by allowing the system to achieve thermal equilibrium, after which the magnetization is calculated dynamically using the atomistic approach with LD. The fluctuations relative to the average magnetization in each case were calculated as $\Delta m(t) = (M_{\rm tot}(t) - \langle M_{\rm tot}\rangle)/\langle M_{\rm tot}\rangle$, with $M_{\rm tot}(t)$ the instantaneous magnitude of the magnetization and $\langle M_{\rm tot}\rangle$ the average. The results for the two cube sizes are given in Fig. 6(a) and (b), respectively. The fluctuations are significant in both cases, but clearly more pronounced in the case of the 1.5 nm cube, which exhibits fluctuations of the magnetization of 10%–15%.

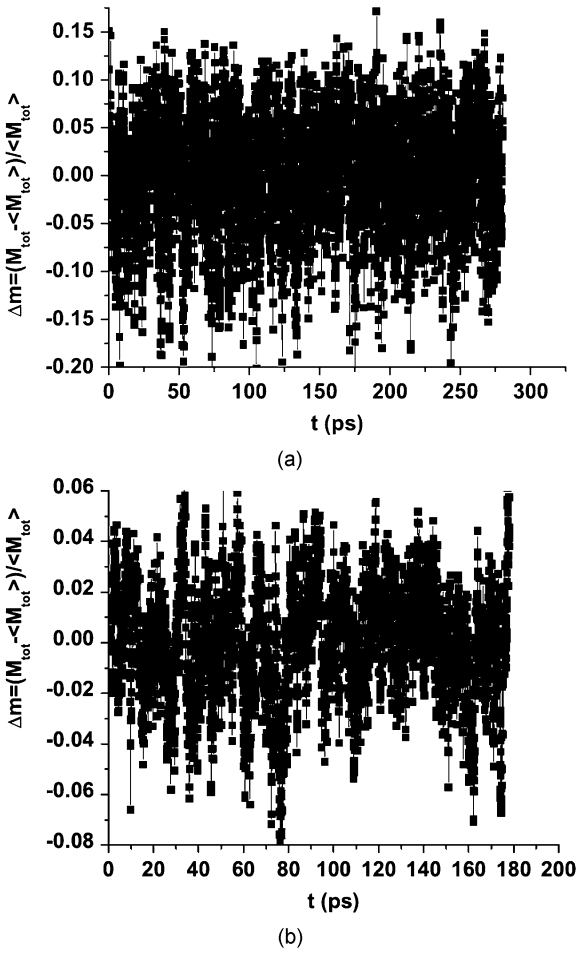

Fig. 6. Magnetization fluctuations for (a) a $1.5 \times 1.5 \times 1.5$ nm, and (b) a $3 \times 3 \times 3$ nm Fe cube.

It is interesting to consider the implications of these calculations for dynamic simulations of both micromagnetic systems and nanoparticles. In each case, treating the moment as a single spin allows the use of the LLG equation in its usual form (3). However, the LLG equation allows only transverse fluctuations of the magnetization, in which the magnitude of the magnetization remains constant. Longitudinal fluctuations of the magnetization can be introduced via the Bloch form of damping,

leading to the Landau–Lifshitz–Bloch (LLB) equation, which has the following form for the longitudinal relaxation:

$$\frac{d\hat{m}_z}{dt} = (\hat{m} - \hat{m}_z)/\tau_1 \tag{5}$$

where τ_1 is the longitudinal relaxation time. The transverse equation of motion is

$$\frac{d\hat{m}_{x,y}}{dt} = -(||\gamma_0||\hat{m} \times \vec{H})_{x,y} - \hat{m}_{x,y}/\tau_2. \tag{6}$$

The LLB equation does not conserve the magnitude of the magnetization, except for the special case $\tau_2 = 2\tau_1$, and may be more appropriate for applications in nanoparticle dynamics and in micromagnetic simulations with extremely fine discretizations. Garanin and Fesenko [15] have recently introduced thermal activation into the LLB equation, leading to a formalism capable of simulating thermally activated magnetization reversal and magnetization fluctuations. A detailed analysis of our dynamic data in terms of the LLB equation is beyond the scope of this paper and will be published elsewhere, but it is important to note that the LLB equation represents an intriguing alternative to the LLG equation, in that it does allow the longitudinal fluctuations along with any impact they might have on long-wavelength fluctuations.

V. Conclusion

In this paper, we have explored the limits of the micromagnetic formalism arising from the use of a continuum approach and the consequent long-wavelength approximation to the exchange which is introduced as a necessary compromise. It is argued that some form of atomistic approach is necessary for read elements as they decrease in thickness to values around 1.5 nm as recording densities of 1 Tb/in^2 are approached. Ultimately, the need is to introduce the short-wavelength fluctuations of the magnetization which are responsible for the ferromagnetic/paramagnetic phase transition. This has also been the subject of work by Grinstein and Koch [16]. Here, we have used a relatively simple computational approach which, being based at the atomic level, has all the features of the analytical approaches. In our case, the challenge is to develop accurate techniques for the magnetostatic field term. Here, we outline an approach based on the use of a superlattice of "macrocells" imposed on the computational cell. Within each macrocell, the magnetization is averaged and the supercell of averaged spins used to calculate the magnetostatic field.

The results of the calculations demonstrate several important finite size effects which are not accessible to micromagnetic calculations. These include a loss of surface magnetization in 1.5-nm-thick films. In terms of finite size effects we have also found that interface mixing leads to an effective reduction of the Curie temperature resulting in increased magnetic noise due to larger magnetization fluctuations [17] and the observation of longitudinal fluctuations of the magnetization, which suggest that the LLB equation could be appropriate for the description of damping in small particles and micromagnetic systems with small discretization lengths. The results suggest that it is not only realistically possible to develop an atomistic model of a read sensor, but also that there are strong indications that such a development is important, since the finite size effects revealed here must be dealt with at the atomistic level. Our results also show that it is possible to simulate pump–probe experiments, which naturally involve a change in the magnetization arising from laser-induced temperature variations. This is difficult with a purely micromagnetic model given that such models do not correctly predict the temperature variation of the magnetization.

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